

# The Poisson equation at second order in relativistic cosmology

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(Dated: March 14, 2013)

We calculate the relativistic constraint equation which relates the curvature perturbation to the matter density contrast at second order in cosmological perturbation theory. This relativistic “second order Poisson equation” is presented in a gauge where the hydrodynamical inhomogeneities coincide with their Newtonian counterparts exactly for a perfect fluid with constant equation of state. We use this constraint to introduce primordial non-Gaussianity in the density contrast in the framework of General Relativity. We then derive expressions that can be used as the initial conditions of N-body codes for structure formation which probe the observable signature of primordial non-Gaussianity in the statistics of the evolved matter density field.

PACS numbers: 98.80.Cq

## I. INTRODUCTION

Our knowledge of the statistics of the galaxy distribution relies upon the vast amount of data obtained by increasingly large galaxy surveys [1–4]. Among other goals, analysis of the galaxy field allows us to indirectly probe the distribution of the underlying dark matter on non-linear scales (e.g., Refs. [5, 6]). On the theoretical side, in order to understand the physics that governs the observed galaxy field, large numerical codes are developed to simulate the evolution of matter inhomogeneities that have formed large scale structure (LSS). This huge task is usually split in two stages. In a first stage, semi-analytical methods are employed to account for the early evolution of fluctuations in the weakly non-linear regime. At the same time, the inhomogeneous in the continuum matter field are related to a discrete distribution of point masses, thus implementing initial conditions for numerical codes. In a second stage, typically at redshifts  $z \sim 50$ , N-body codes evolve inhomogeneities in the strongly non-linear regime up to the present day. As Newtonian N-body codes continue to improve in resolution and volume (e.g., Refs. [7–9]), the implementation of realistic and accurate initial conditions is increasingly important.

Historically, the initial conditions for N-body simulations have been generated by using the Zel’dovich approximation [10], which establishes the correspondence between the matter density fluctuation of standard perturbation theory, and the displacement of mass particles in a grid. Despite its linear nature, this represents an improvement over standard perturbation theory, since it takes advantage of working in Lagrangian coordinates [6, 11]. The caveat to this approximation is that it accounts only for the early non-linear evolution of density fluctuations, and in particular, it employs a linear Poisson constraint, which is used to express the density contrast,  $\delta_N$ , in terms of the gravitational potential,  $\phi_N$ , that is

$$\nabla^2 \phi_N = 4\pi G \rho_0 a^2 \delta_N. \quad (1.1)$$

An improvement to this approximation is second-order Lagrangian perturbation theory (2LPT), which generates initial conditions taking into account non-linearities in Lagrangian coordinates. This has been shown to be more precise and avoids transients present in the Zel’dovich approximation [12, 13]. Since 2LPT takes into account non-linearities, the fact that the gravitational instability is non-local is manifest in corrections to Eq. (1.1) given by tidal effects at non-linear order [14]. With the matter density fluctuations at non-linear order under control, recent studies have used 2LPT to include primordial non-Gaussianity in the matter fluctuations [15–17].

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These and other semi-analytical approximations to the early evolution of inhomogeneities, however, rely on Newtonian physics, thereby ignoring the effects of General Relativity (GR). Cosmological inhomogeneities are well described by Newtonian dynamics only when the modes of the perturbations lie well inside the horizon, i.e. when their wavenumber is  $k \gg \mathcal{H}$ , with  $\mathcal{H}$  denoting the Hubble parameter in conformal time. Yet, the initial conditions for these approximations come from much earlier times –typically the epoch of decoupling–, when some of the scales of interest are comparable to, or even larger than, the cosmological horizon. Therefore, relativistic effects are important and should be taken into account when setting the initial conditions to simulations of structure formation.

Recent studies demonstrate the importance of GR in the analysis of large scale structure. Some have contrasted relativistic and Newtonian fluctuations by the identification of dynamical equations [18, 19]. This provides correspondences between Newtonian fluctuations and relativistic perturbations in a specific gauge at linear order in perturbation theory. Additionally, Ref. [20] extends this correspondences to second-order perturbations. In this way, the equivalence of the dynamical equations is established for the restricted case of pressureless matter and neglecting the decaying mode of perturbations. A major motivation to study this correspondence is to discriminate primordial non-Gaussian fluctuations from non-Gaussianities induced by the non-linear dynamics of GR. In search of observational signatures, Ref. [21] studied the effects of relativistic non-linear fluctuations in the halo bias and subsequently its signature in the spectrum of the galaxy distribution (see also [22]).

In this paper we present the Poisson equation at second order in the framework of relativistic cosmological perturbation theory [23–27]. Previous studies have explored this constraint for the limit of a dust universe at small scales [20] (in this case the linear equation (1.1) is recovered), and for a  $\Lambda$ CDM universe at large scales [28]. Instead, our analysis yields the Poisson constraint equation in terms of relativistic perturbations that find a direct correspondence with Newtonian inhomogeneities, and without approximations. Furthermore, we extend the constraint to the case of a general perfect fluid. As an example, we subsequently use our result to express the primordial non-Gaussianity in terms of the dark matter density field in equations that include all the relativistic effects. We present results in the form of kernels for the non-linear variables, a form customarily used in the formulation of initial conditions of numerical simulations.

The paper is organised as follows. In the next section we explicitly show how to construct the Poisson equation from Einstein’s field equations combining variables in two gauges for linear perturbations. In Section III we repeat the procedure for the second order variables and arrive at a GR version of the Poisson constraint valid for any perfect fluid including entropy (or non-adiabatic pressure) perturbations. In Section IV we apply the constraint to the case of matter perturbations in a flat universe dominated by pressureless matter and show how to include the primordial non-Gaussian corrections in the Poisson equation. We conclude in Section V discussing the relevance of our result to the initial conditions of numerical simulations.

## II. THE POISSON EQUATION AT FIRST ORDER

### A. Background and first-order equations

In cosmological perturbation theory, considering scalar perturbations of the metric yields the following line element,

$$ds^2 = a^2(\eta) \left\{ -(1 + 2\phi)d\eta^2 + 2B_{,i}dx^i d\eta + \left[ (1 - 2\psi)\delta_{ij} + E_{,ij} \right] dx^i dx^j \right\}, \quad (2.1)$$

where  $\phi$  is the lapse function,  $\psi$  is the curvature perturbation, and  $B$  and  $E$  make up the scalar shear. All these quantities are function of Cartesian coordinates,  $x_j$ , and conformal time,  $\eta$ . Perturbations are then expanded order-by-order in a series as, e.g.,  $\phi = \phi_1 + \frac{1}{2}\phi_2 + \dots$ . In order to define the expansion uniquely, and as an excellent approximation to observations, the first order quantities are chosen to have Gaussian statistics.

In the background the metric represents the Friedmann-Lemaître-Robertson-Walker spacetime. The homogeneous equations are the familiar Friedmann and continuity equations:

$$3\mathcal{H}^2 = 8\pi G\rho_0, \quad (2.2)$$

$$\rho'_0 = -3\mathcal{H}(P_0 + \rho_0), \quad (2.3)$$

where the prime denotes a derivative with respect to conformal time and a subscript zero denotes the background, homogeneous quantities.

The fluid equations are derived from the vanishing covariant derivative of the energy momentum tensor. At first-order in perturbation theory, the energy conservation dictates the evolution of the density perturbation  $\delta\rho_1$ ,

$$\delta\rho'_1 + 3\mathcal{H}(\delta\rho_1 + \delta P_1) = (\rho_0 + P_0) [3\psi'_1 - \nabla^2(E'_1 + v_1)], \quad (2.4)$$

where the scalar velocity potential is  $v(x^j, t)$  and the energy density and pressure fluctuations are denoted by  $\delta\rho$  and  $\delta P$ , respectively. We define the Laplacian as  $\nabla^2 = \partial_j \partial^j$ . Note that no gauge has been specified here. In order to obtain the corresponding equation for the evolution of the velocity, we define  $V = B + v$ , and write the momentum conservation equation, which at first order is

$$V'_{1,i} + \mathcal{H}(1 + c_s^2)V_{1,i} + \left[ \frac{\delta P_1}{P_0 + \rho_0} + \phi_1 \right]_{,i} = 0, \quad (2.5)$$

where we have neglected anisotropic stresses and defined the adiabatic sound speed as  $c_s^2 = P'_0/\rho'_0$ .

The Einstein field equations yield two constraint equations that are combined to derive the Poisson equation. The  $(0, 0)$  component of these equations yields the energy constraint equation

$$3\mathcal{H}(\psi'_1 + \mathcal{H}\phi_1) - \nabla^2(\psi_1 + \mathcal{H}(E'_1 - B_1)) = -4\pi G a^2 \delta\rho_1. \quad (2.6)$$

The momentum constraint is derived from the  $(0, i)$  component:

$$\psi'_{1,i} + \mathcal{H}\phi_{1,i} = -4\pi G a^2 (\rho_0 + P_0)V_{1,i}. \quad (2.7)$$

This is the complete set of equations at first order without the gauge specified. The remaining Einstein equations at this order are related to the ones above through the Bianchi identities.

### B. Constraint in the longitudinal gauge

In order to overcome the ambiguity in the coordinate freedom, we must specify the gauge in the above equations. We work in the longitudinal or Newtonian gauge [23] to recover the exact Newtonian equations. This is a shear-free gauge, specified by setting  $E_\ell = B_\ell = 0$ . The absence of anisotropic stresses also guarantees that, in this gauge,  $\psi_{1\ell} = \phi_{1\ell}$  and Eq. (2.6) becomes

$$-3\mathcal{H}(\phi'_{1\ell} + \mathcal{H}\phi_{1\ell}) + \nabla^2\phi_{1\ell} = 4\pi G a^2 \delta\rho_{1\ell}. \quad (2.8)$$

Then, by integrating the overall gradient of the momentum constraint (2.7), we have

$$\phi'_{1\ell} + \mathcal{H}\phi_{1\ell} = -4\pi G a^2 (\rho_0 + P_0)v_{1\ell}, \quad (2.9)$$

and combining both equations we find the first-order constraint:

$$\nabla^2\phi_{1\ell} = 4\pi G a^2 (\delta\rho_{1\ell} + \rho'_0 v_{1\ell}). \quad (2.10)$$

### C. The Newtonian expression

The quantity in parenthesis in the linear Poisson equation (2.10), is equivalent to the density contrast in two other gauges as we will now show. The transformation between two coordinate systems is carried through the four-vector  $\xi_{1\mu} = (\alpha_1, \beta_{1,i})$ , so that, for example, the density perturbation at linear order is transformed as

$$\widetilde{\delta\rho_1} = \delta\rho_1 + \alpha\rho'_0. \quad (2.11)$$

The total matter gauge is defined by a vanishing total momentum at all orders, i.e.

$$\widetilde{V_{\text{tom}}} = 0. \quad (2.12)$$

The transformation rule for  $V$  tells us that

$$\widetilde{V_1} \equiv \widetilde{v_1} + \widetilde{B_1} = v_1 + B_1 - \alpha_1, \quad (2.13)$$

so that in the case of a transformation from the longitudinal to the total matter gauge we have

$$\alpha_{1\text{tom}} = v_{1\ell}. \quad (2.14)$$

In consequence, the density fluctuation is obtained as

$$\widetilde{\delta\rho_{1\text{tom}}} = \delta\rho_{1\ell} + \rho'_0 v_{1\ell}. \quad (2.15)$$

It is now straightforward to recover the Newtonian form of the Poisson equation writing

$$\nabla^2 \phi_{1\ell} = 4\pi G a^2 \rho_0 \delta_{1\text{tom}}, \quad (2.16)$$

where the density contrast is, at first order,  $\delta_{1\text{tom}} = \delta\rho_{1\text{tom}}/\rho_0$ , and at second order  $\delta_{2\text{tom}} = \delta\rho_{2\text{tom}}/\rho_0$ .

An equivalent transformation can be performed to arrive at the comoving gauge, where the shear is vanishing and  $B_{\text{com}} = E_{\text{com}} = v_{\text{com}} = 0$ . In this case, one finds that  $\alpha_{\text{com}} = v_\ell$ , just as in the total matter gauge. Thus, the matter density at linear order  $\delta\rho_{1\text{com}}$  reproduces the expression in (2.14). The corresponding Poisson equation

$$\nabla^2 \phi_{1\ell} = 4\pi G a^2 \rho_0 \delta_{1\text{com}}, \quad (2.17)$$

has been recovered in previous works [5, 29]. It has further been shown that with the same combination of variables (namely  $\delta_{1\text{com}}, \phi_{1\ell}, v_\ell$ ) one can reproduce the equations used in Newtonian hydrodynamics at linear order [18, 19], with the exception of fluids with non-vanishing pressure, and which allow for entropy perturbations [30]. At second order, however, the gauge transformation  $\delta_{2\ell} \rightarrow \delta_{2\text{com}}$  include time integrals which may introduce non-local terms. We avoid such complication here by working with the matter fluctuation in the total matter gauge. For the sake of completeness, we construct the scalar  $\beta_{\text{tom}}$ , which is determined by the transformation  $E_{1\text{tom}} = E_{1\ell} + \beta_{1\text{tom}} = 0$ , that is

$$\beta_{1\text{tom}} = 0. \quad (2.18)$$

### III. THE CONSTRAINT AT SECOND ORDER

In the previous section we have shown how the linear energy and momentum constraint equations can be combined to obtain a Poisson equation at first order. The same procedure can be followed to write a Poisson-like constraint at second order, although the manipulation of terms is obviously more complicated.

#### A. Second-order equations

The energy constraint at second order in a non-specific gauge form is [31],

$$\begin{aligned} & 3\mathcal{H}(\psi_2' + \mathcal{H}\phi_2) + \nabla^2 \left( \mathcal{H}(B_2 - E_2') - \psi_2 \right) + \nabla^2 B_1 \left( \nabla^2 (E_1' - \frac{1}{2}B_1) - 2\psi_1' \right) \\ & + B_{1,i} \left( \mathcal{H}(3\mathcal{H}B_{1,i} - 2\nabla^2 E_{1,i} - 2(\psi_1 + \phi_1)_{,i}) - 2\psi_{1,i}' \right) + 2E_{1,ij} (\psi_1 - 2\mathcal{H}B_1)_{,ij} \\ & + 4\mathcal{H}(\psi_1 - \phi_1) \left( 3\psi_1' - \nabla^2 (E_1' - B_1) \right) + E_{1,ij} \left( 4\mathcal{H}E_1 + \frac{1}{2}E_1' - B_1 \right)_{,ij} \\ & + \psi_1' \left( 2\nabla^2 (E_1' - 2\mathcal{H}E_1) - 3\psi_1' \right) + \psi_{1,i} (2\nabla^2 E_1 - 3\psi_1)_{,i} + 2\nabla^2 \psi_1 (\nabla^2 E_1 - 4\psi_1) \\ & - 12\mathcal{H}^2 \phi_1^2 + \frac{1}{2} \left( B_{1,ij} B_{1,ij} + \nabla^2 E_{1,j} \nabla^2 E_{1,j} - E_{1,ijk} E_{1,ijk} - \nabla^2 E_1' \nabla^2 E_1' \right) \\ & = -4\pi G a^2 \left( 2(\rho_0 + P_0) V_{1,k} v_{1,k} + \delta\rho_2 \right), \end{aligned} \quad (3.1)$$

while the momentum constraint is

$$\begin{aligned} & \psi_{2,i}' + \mathcal{H}\phi_{2,i} - E_{1,ij}' (\psi_1 + \phi_1 + \nabla^2 E_1)_{,j} + B_{1,ij} (2\mathcal{H}B_1 + \phi_1)_{,j} \\ & - \left[ \psi_{1,i} (\nabla^2 E_1 - 4\psi_1) \right]' - \phi_{1,i} \left( 8\mathcal{H}\phi_1 + 2\psi_1' + \nabla^2 (E_1' - B_1) \right) \\ & - B_{1,j} \psi_{1,i}{}^{,j} + 2\psi_{1,i}' E_{1,ij} + E_{1,jk}' E_{1,i}{}^{,jk} - \psi_{1,i}' (\nabla^2 E_1 + 4\phi_1) - \nabla^2 \psi_1 B_{1,i} \\ & = -4\pi G a^2 \left[ (\rho_0 + P_0) \left( V_{2,i} - 2\phi_1 (V_1 + B_1)_{,i} - 4(\psi_1 v_{1,i} - E_{1,ik} v_{1,k}) \right) \right. \\ & \quad \left. + 2(\delta\rho_1 + \delta P_1) V_{1,i} \right]. \end{aligned} \quad (3.2)$$

Both equations are simplified by choosing a gauge. In the longitudinal gauge (incidentally called Poisson gauge at second order when one ignores the vector and tensor modes), Eq. (3.1) takes the form

$$\begin{aligned} & 3\mathcal{H}(\psi'_{2\ell} + \mathcal{H}\phi_{2\ell}) - \nabla^2\psi_{2\ell} - 3\phi_{1\ell}^{\prime 2} - 3\phi_{1\ell,k}\phi_{1\ell}^{\prime,k} - 8\phi_{1\ell}\nabla^2\phi_{1\ell} - 12\mathcal{H}^2\phi_{1\ell}^2 \\ & = -4\pi Ga^2\rho_0\left(\delta\rho_{2\ell} + 2(1+w)v_{1\ell}^{\prime,k}v_{1\ell,k}\right), \end{aligned} \quad (3.3)$$

while Eq. (3.2) is reduced to

$$\begin{aligned} & (\psi'_{2\ell} + \mathcal{H}\phi_{2\ell})_{,i} + 2(\phi_{1\ell,i}\phi_{1\ell})' - 8\mathcal{H}\phi_{1\ell,i}\phi_{1\ell} - 2\phi_{1\ell,i}'\phi_{1\ell} \\ & = -4\pi Ga^2\rho_0\left\{(1+w)[v_{2\ell,i} - 6v_{1\ell,i}\phi_{1\ell}] + 2(1+c_s^2)v_{1\ell,i}\delta_{1\ell} + 2\frac{1}{\rho_0}\delta P_{\text{nad1}}v_{1\ell,i}\right\}. \end{aligned} \quad (3.4)$$

Here  $w = P_0/\rho_0$  is the equation of state of the fluid, and the non-adiabatic pressure perturbation,  $\delta P_{\text{nad1}}$ , is defined as

$$\delta P_{\text{nad1}} = \delta P_1 - c_s^2\delta\rho_1. \quad (3.5)$$

Following the steps of the procedure at first order, we take the spatial divergence of Eq. (3.4) and integrate with the inverse Laplacian operator  $\nabla^{-2}$ . We obtain

$$\begin{aligned} & \psi'_{2\ell} + \mathcal{H}\phi_{2\ell} + (\phi_{1\ell}^2)' - 4\mathcal{H}\phi_{1\ell}^2 - 2\nabla^{-2}(\phi_{1\ell,j}'\phi_{1\ell})^j \\ & = -4\pi Ga^2\rho_0\left\{(1+w)\left[v_{2\ell} - 6\nabla^{-2}(v_{1\ell,j}\phi_{1\ell})^j\right] + 2(1+c_s^2)\nabla^2(v_{1\ell,j}\delta_{1\ell})^j + 2\frac{1}{\rho_0}(\delta P_{\text{nad1}}v_{1\ell,j})^j\right\}. \end{aligned} \quad (3.6)$$

We can now substitute this into Eq. (3.3) to arrive at

$$\begin{aligned} & \nabla^2\psi_{2\ell} + 3(\phi_{1\ell}')^2 + \frac{3}{2}\nabla^2(\phi_{1\ell}^2) + 5\phi_{1\ell}\nabla^2\phi_{1\ell} + 3\mathcal{H}(\phi_{1\ell}^2)' - 6\mathcal{H}\nabla^2[\phi_{1\ell,j}'\phi_{1\ell}]^j \\ & = 4\pi Ga^2\rho_0\left\{\delta_{2\ell} - 3\mathcal{H}(1+w)v_{2\ell} + 2(1+w)v_{1\ell,j}v_{1\ell}^{\prime,j} + 6\mathcal{H}\nabla^{-2}\left[v_{1\ell,j}\left(3(1+w)\phi_{1\ell} - (1+c_s^2)\delta_{1\ell} - \frac{1}{\rho_0}\delta P_{\text{nad1}}\right)\right]^j\right\} \end{aligned} \quad (3.7)$$

## B. The Poisson equation at second order

To write the second-order equivalent of the Poisson equation in (2.16), we must transform the density contrast to the total matter gauge. The transformation rule at second order is [26]

$$\widetilde{\delta\rho_{2\text{tom}}} = \delta\rho_{2\ell} + \rho_0'\alpha_{2\text{tom}} + \alpha_{1\text{tom}}(\rho_0''\alpha_{1\text{tom}} + \rho_0'\alpha_{1\text{tom}}' + 2\delta\rho_{1\ell}'). \quad (3.8)$$

The second-order  $\alpha_{2\text{tom}}$  evaluated in the longitudinal gauge is found with the aid of expressions in Ref. [31],

$$\alpha_{2\text{tom}} = v_{2\ell} - \mathcal{H}v_{1\ell}^2 + \frac{1}{2}(v_{1\ell}^2)' - 4\nabla^2[v_{1\ell,j}(\phi_{1\ell} - v_{1\ell}')^j]. \quad (3.9)$$

With the aid of the background equations and the expressions for  $\alpha_{1\text{tom}}$  in Eq. (2.14) and  $\delta_{1\text{tom}}$  in Eq. (2.15) we obtain the gauge transformation,

$$\begin{aligned} \widetilde{\delta_{2\text{tom}}} & = \delta_{2\ell} - 3\mathcal{H}(1+w)v_{2\ell} - 3\mathcal{H}(1+w)v_{1\ell}\delta_{1\text{tom}} + 2v_{1\ell}\delta_{1\text{tom}}' \\ & \quad + 12\mathcal{H}(1+w)\nabla^{-2}[v_{1\ell,j}(\phi_{1\ell} + v_{1\ell}')^j] + \left[3\mathcal{H}w' - \frac{3}{2}\mathcal{H}^2(1+w)(5+9w)\right]v_{1\ell}^2. \end{aligned} \quad (3.10)$$

We substitute the  $\delta_\ell$  factors at both orders into Eq. (3.7) for the total matter gauge equivalents. The final expression in terms of  $\delta_{\text{tom}}$ ,  $\phi_{1\ell}$  and  $v_{1\ell}$  is then

$$\begin{aligned} & \nabla^2\psi_{2\ell} + 3(\phi_{1\ell}')^2 + \frac{3}{2}\nabla^2(\phi_{1\ell}^2) + 5\phi_{1\ell}\nabla^2\phi_{1\ell} + 3\mathcal{H}(\phi_{1\ell}^2)' - 6\mathcal{H}\nabla^{-2}[\phi_{1\ell}\phi_{1\ell,j}']^j \\ & = 4\pi Ga^2\rho_0\left\{\delta_{2\text{tom}} + 6\mathcal{H}(1+w)v_{1\ell}\delta_{1\text{tom}} - 2v_{1\ell}\delta_{1\text{tom}}' + 2(1+w)v_{1\ell,j}v_{1\ell}^{\prime,j} + \frac{3}{2}\mathcal{H}^2(1+w)(3w-1)v_{1\ell}^2\right. \\ & \quad \left.+ 6\mathcal{H}(1+w)\nabla^{-2}\left[v_{1\ell,j}\left(\phi_{1\ell} - 2v_{1\ell}' - \left(\frac{1+c_s^2}{1+w}\right)\delta_{1\text{tom}} - \frac{1}{1+w}\frac{\delta P_{\text{nad1}}}{\rho_0}\right)\right]^j\right\}. \end{aligned} \quad (3.11)$$

This rather long equation fulfils our first goal, to provide a Poisson equation at second order using the same variables employed in the structure formation studies at the Newtonian limit. It is already clear that adopting the expression  $\nabla^2 \psi_2 = 4\pi G a^2 \rho_0 \delta_2$  leaves out most of the terms of the actual second order Poisson constraint.

To conclude this section, let us rewrite Eq. (3.11) in terms of the potential  $\phi_{2\ell}$  instead of  $\psi_{2\ell}$ . This will come handy in the next section since primordial non-Gaussianity is conventionally formulated in terms of this variable. We use the traceless  $ij$  component of the field equations as

$$\begin{aligned} \nabla^4(\psi_{2\ell} - \phi_{2\ell}) = & -4\nabla^4(\phi_{1\ell}^2) + 2\phi_{1\ell,j}^i \phi_{1\ell,i}^j + 6\nabla^2\phi_{1\ell}\nabla^2\phi_{1\ell} + 8\phi_{1\ell,j}\nabla^2\phi_{1\ell,j} \\ & + 4\pi G a^2 \rho_0 \left\{ 2(1+w) \left[ \nabla^2(v_{1\ell,j}v_{1\ell}^j) + 3\nabla^2(v_{1\ell}\nabla^2v_{1\ell}) + 3\nabla^2(v_{1\ell})\nabla^2(v_{1\ell}) - 3v_{1\ell}\nabla^4v_{1\ell} \right] \right\}. \end{aligned} \quad (3.12)$$

Upon substitution of this in the constraint equation, Eq. (3.11), and with some algebra we arrive at

$$\begin{aligned} & \nabla^4\phi_{2\ell} - 2\nabla^4(\phi_{1\ell}^2) + 7\nabla^2(\phi_{1\ell}\nabla^2\phi_{1\ell}) + 3(\nabla^2\phi_{1\ell})^2 - 3\phi_{1\ell}\nabla^4\phi_{1\ell} + 3\nabla^2(\phi_{1\ell}'^2) + 3\mathcal{H}\nabla^2\phi_{1\ell}' - 6\mathcal{H}(\phi_{1\ell,j}'\phi_{1\ell}^j), \\ & = 4\pi G a^2 \rho_0 \left\{ \nabla^2\delta_{2\text{tom}} + 6\mathcal{H}(1+w)\nabla^2(v_{1\ell}\delta_{1\text{tom}}) - 2\nabla^2(v_{1\ell}\delta_{1\text{tom}}') + \frac{3}{2}\mathcal{H}^2(1+w)(3w-1)\nabla^2v_{1\ell}^2 \right. \\ & \left. + 6(1+w) \left[ v_{1\ell}\nabla^4v_{1\ell} - \nabla^2(v_{1\ell}\nabla^2v_{1\ell}) - (\nabla^2v_{1\ell})^2 + \mathcal{H} \left( v_{1\ell,j} \left( \phi_{1\ell} - 2v_{1\ell}' - \frac{1+c_s^2}{1+w}\delta_{1\text{tom}} - \frac{1}{1+w}\frac{\delta P_{\text{nad1}}}{\rho_0} \right) \right)^j \right] \right\}. \end{aligned} \quad (3.13)$$

This constraint is valid for any perfect fluid. In the following section we show how to insert this constraint in the initial conditions of numerical simulations of structure formation.

#### IV. NON-GAUSSIAN INITIAL CONDITIONS FOR NUMERICAL SIMULATIONS

The Newtonian Poisson equation is used at all orders as a constraint to the initial conditions in numerical simulations. However, the above constraint is the one that provides consistency with General Relativity. Imposed at an initial time, this constraint is met at all times if the perturbations are evolved in the context of GR. It is therefore useful to write the expression we have derived in terms of variables employed in numerical simulations, namely  $\delta_{1\text{tom}}$  and  $v_{1\ell}$ , evaluated at some initial time. Here we derive such an expression with the aid of the first order equations, Eqs. (2.9), (2.16), and the continuity equation from Ref. [30] in terms of the chosen gauge. These help us to replace the time derivatives in the constraint equations. After some more algebra we obtain

$$\begin{aligned} & \nabla^4\phi_{2\ell} - 2\nabla^4(\phi_{1\ell}^2) + 7\nabla^2(\phi_{1\ell}\nabla^2\phi_{1\ell}) + 3(\nabla\phi_{1\ell})^2 - 3\phi_{1\ell}\nabla^4\phi_{1\ell} \\ & = 4\pi G a^2 \rho_0 \left\{ \nabla^2\delta_{2\text{tom}} + 6(1+w) \left[ v_{1\ell}\nabla^4v_{1\ell} - (\nabla^2v_{1\ell})^2 - \frac{2}{3}\nabla^2(v_{1\ell}\nabla^2v_{1\ell}) + \frac{3}{4}(1+w)\mathcal{H}^2\nabla^2(v_{1\ell}^2) \right] \right. \\ & \left. + 6\mathcal{H}\nabla^2(v_{1\ell}\delta_{1\ell}) + 6(1+w)\mathcal{H} \left[ v_{1\ell,j} \left( 2\phi_{1\ell} - \frac{c_s^2-1}{1+w}\delta_{1\text{tom}} + \frac{1}{1+w}\frac{\delta P_{\text{nad1}}}{\rho_0} \right) \right]^j \right\}. \end{aligned} \quad (4.1)$$

We emphasise that the Newtonian counterpart of this constraint is a linear equation which includes only the first term at each side of the equality. All the other terms bring relativistic contributions to the Poisson equation. This expression can be used in the numerical simulations that set initial conditions for perturbations of in any perfect fluid and allowing for entropy perturbations.

To reduce Eq. (4.1) further, we can either eliminate the density contrast  $\delta_{1\text{tom}}$  or the potential  $\phi_{1\ell}$  via the first-order Poisson equation (2.16). This proves useful when we want to make contact with formulations like the so-called renormalised perturbation theory (RPT)[32], where the initial conditions are set, order by order in Fourier space, via recursive relations in powers of  $\delta_{1\text{N}}$  (see, e.g., Ref. [6]). To reduce things further, let us focus on the case of an Einstein-de Sitter universe, a flat space-time filled by dust, i.e., where  $w = 0$  as well as  $\delta P_1 = 0$  and  $\Lambda = 0$ . In this case, Eq. (4.1) is reduced to

$$\begin{aligned} & \nabla^4\phi_{2\ell} - 2\nabla^4(\phi_{1\ell}^2) + 7\nabla^2\phi_{1\ell}\nabla^2\phi_{1\ell} - 3\phi_{1\ell}\nabla^4\phi_{1\ell} + 3(\nabla^2\phi_{1\ell})^2 \\ & = 4\pi G \rho_0 \left\{ \nabla^2\delta_{2\text{tom}} + \frac{9}{2}\mathcal{H}^2\nabla^2v_{1\ell}^2 + 2 \left[ 3v_{1\ell}\nabla^4v_{1\ell} - 3(\nabla^2v_{1\ell})^2 - 2\nabla^2(v_{1\ell}\nabla^2v_{1\ell}) \right] \right. \\ & \left. + 6\mathcal{H}\nabla^2(v_{1\ell}\delta_{1\ell}) + 6\mathcal{H} \left[ v_{1\ell,j} (2\phi_{1\ell} - \delta_{1\text{tom}}) \right]^j \right\}. \end{aligned} \quad (4.2)$$

With the aim of incorporating our result as an initial constraint in the formulation of non-linear initial conditions for numerical simulations, we transform Eq. (4.2) to the Fourier space. Additionally, as is customary in structure formation studies, we work exclusively with the growing mode of perturbations, where  $\phi_{1\ell} = \text{const.}$  It is then possible to write all of first order variables in terms of  $\delta_{1\text{tom}}$  (as in the standard perturbation theory, c.f. Ref. [6]) with the aid of the first order Poisson equation (2.16) and the continuity equation at first order. Explicitly, in Fourier space,

$$\phi_{1\ell}(k) = -\frac{3}{2} \frac{\mathcal{H}^2}{k^2} \delta_{1\text{tom}}(k), \quad v_{1\ell}(k) = \frac{\mathcal{H}}{k^2} \delta_{1\text{tom}}(k), \quad (4.3)$$

The reduced Poisson equation is

$$k^4 \phi_{2\ell}(k) + \frac{3}{2} k^2 \mathcal{H}^2 \delta_{2\text{tom}}(k) = \frac{3}{2} \int d^3p d^3q \delta_D^3(p+q-k) \frac{\mathcal{H}^4}{p^2 q^2} \times \left\{ 3|p+q|^4 + \frac{15}{4}(p^4 + q^4) - \frac{35}{4}|p+q|^2(p^2 + q^2) - \frac{15}{2}p^2 q^2 + \frac{9}{2}\mathcal{H}^2|p+q|^2 \right\} \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q), \quad (4.4)$$

where  $\delta_D(k)$  is the Dirac delta function. This equation represents a concrete constraint for initial conditions of numerical simulations, consistent with GR, and written in terms of relativistic equivalents to the gravitational potential and the matter density perturbation. Note that, while the linear equation of Ref. [20] is valid for these second order variables at small scales, the relativistic corrections obtained here become increasingly important as the perturbation modes approach the horizon scale.

Since this constraint already carries couplings between different perturbation modes, there will be some *intrinsic* non-Gaussianity induced by this second-order correspondence. This is a known effect of GR which has recently been explored in the CMB through the use of second order Boltzmann codes [33–35], and in the matter density field [28]. Here we disentangle the effect of the initial constraint from the influence of the non-linear evolution of perturbations. To observe the type of non-Gaussianity induced by the GR constraint, we introduce three templates that constitute a basis for the non-Gaussian  $\phi_{2\ell}$ . These templates are also a basis to represent the initial conditions of the density contrast with primordial non-Gaussianity, and consistent with GR, for a given model of structure formation.

Following the convention of [36] for the non-Gaussianity in the lapse function, the local template is,

$$\phi_{\ell}^{\text{loc}} = \phi_{\ell G} + f_{\text{NL}}^{\text{loc}} [\phi_{\ell G}^2 - \langle \phi_{\ell G}^2 \rangle]. \quad (4.5)$$

This is preserved in super-horizon scales since  $\phi_{\ell}$  is constant when the universe is filled with dust. Therefore, we can directly substitute the primordial  $\phi_{2\ell}$  in the Poisson constraint (4.4).

In Fourier space, the local bispectrum yields the correspondence

$$\frac{1}{2} \phi_{2\ell}^{\text{loc}}(k) = \frac{9}{4} f_{\text{NL}}^{\text{loc}} \int d^3p d^3q \delta_D^3(p+q-k) \left( \frac{\mathcal{H}^4}{p^2 q^2} \right) \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q), \quad (4.6)$$

and we can generate a kernel for  $\delta_{2\text{tom}}^{\text{loc}}$ ,

$$\frac{k^2}{\mathcal{H}^2} \delta_{2\text{tom}}^{\text{loc}}(k) = \int d^3p d^3q \frac{1}{p^2 q^2} \delta_D^3(p+q-k) \times \left\{ 3(1 - f_{\text{NL}}^{\text{loc}}) |p+q|^4 + \frac{15}{4}(p^4 + q^4) - \frac{35}{4}|p+q|^2(p^2 + q^2) - \frac{15}{2}p^2 q^2 + \frac{9}{2}\mathcal{H}^2|p+q|^2 \right\} \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q). \quad (4.7)$$

Repeating the procedure for the equilateral and orthogonal configurations, we can provide initial conditions for  $\delta_{2\text{tom}}$  in a complete basis for primordial non-Gaussian perturbations. We borrow the templates implemented in Ref. [17]. For the equilateral configuration, this template is

$$\frac{1}{2} k^4 \phi_{2\ell}^{\text{eq}}(k) = \frac{3}{4} f_{\text{NL}}^{\text{eq}} \int d^3p d^3q \delta_D^3(p+q-k) \left( \frac{\mathcal{H}^4}{p^2 q^2} \right) \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q) \times \left\{ -6|p+q|^4 - \frac{3}{2}(p^2 + q^2)|p+q|^2 + 3(p^j + q^j)|p+q|_j^{-1}|p+q|^4 \right\}, \quad (4.8)$$

while in the orthogonal case

$$\frac{1}{2} k^4 \phi_{2\ell}^{\text{ort}}(k) = \frac{3}{4} f_{\text{NL}}^{\text{ort}} \int d^3p d^3q \delta_D^3(p+q-k) \left( \frac{\mathcal{H}^4}{p^2 q^2} \right) \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q) \times \left\{ -21|p+q|^4 + 6(p^2 + q^2)|p+q|^2 + \frac{15}{2}(p^j + q^j)|p+q|_j^{-1}|p+q|^4 \right\}. \quad (4.9)$$

Finally the complementary equilateral and orthogonal kernels for  $\delta_{2\text{tom}}$  are

$$\begin{aligned} \frac{k^2}{\mathcal{H}^2} \delta_{2\text{tom}}^{eq}(k) &= \int d^3p d^3q \frac{1}{p^2 q^2} \delta_D^3(p+q-k) \\ &\times \left\{ 3(1 + 2f_{\text{NL}}^{eq}) |p+q|^4 + \frac{1}{4} (6f_{\text{NL}}^{eq} - 35) |p+q|^2 (p^2 + q^2) - 3f_{\text{NL}}^{eq} |p+q|^4 (p^j + q^j) |p+q|_j^{-1} \right. \\ &\quad \left. + \frac{15}{4} (p^4 + q^4) - \frac{15}{2} p^2 q^2 + \frac{9}{2} \mathcal{H}^2 |p+q|^2 \right\} \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q), \end{aligned} \quad (4.10)$$

$$\begin{aligned} \frac{k^2}{\mathcal{H}^2} \delta_{2\text{tom}}^{ort}(k) &= \int d^3p d^3q \frac{1}{p^2 q^2} \delta_D^3(p+q-k) \\ &\times \left\{ 3(1 + 7f_{\text{NL}}^{ort}) |p+q|^4 - \frac{1}{4} (24f_{\text{NL}}^{ort} + 35) |p+q|^2 (p^2 + q^2) - \frac{15}{2} f_{\text{NL}}^{ort} |p+q|^4 (p^j + q^j) |p+q|_j^{-1} \right. \\ &\quad \left. + \frac{15}{4} (p^4 + q^4) - \frac{15}{2} p^2 q^2 + \frac{9}{2} \mathcal{H}^2 |p+q|^2 \right\} \delta_{1\text{tom}}(p) \delta_{1\text{tom}}(q). \end{aligned} \quad (4.11)$$

The set of these three kernels are a complete basis for the primordial bispectrum. The kernels above show that the Poisson constraint yields different contributions for the local, equilateral and orthogonal configurations. The relativistic initial conditions can mimic non-Gaussian contributions, which peak in the local configuration. This relativistic intrinsic non-Gaussian imprint in the matter fluctuation has a maximum in the local template where  $f_{\text{NL}}^{loc(GR)} = -1$  ( $f_{\text{NL}}^{loc}$  is particularly relevant in studies of LSS since it is the dominant configuration contributing to the dark matter halo bias [37]). In the equilateral configuration, we find that the intrinsic GR imprints are  $f_{\text{NL}}^{eq(GR)} = 1/2$ .

The result obtained for the intrinsic non-Gaussianity is close to that in Ref. [28] which indicates a value in the local configuration of  $f_{\text{NL}}^{loc(GR)} = -5/3$ . The difference is most likely due to a choice of the variable in which the result is expressed. A detailed analysis of the modification of  $f_{\text{NL}}$  separating initial constraints from the non-linear evolution of  $\delta_2$  is the subject of a forthcoming paper [38].

## V. DISCUSSION

In this paper we have derived the relationship between the energy density fluctuation and the curvature perturbation at second order in the context of cosmological perturbation theory. This Poisson equation at second order, presented in Eq. (4.1) in full generality for a single fluid including entropy perturbations, is expressed in terms of variables equivalent to an Eulerian set in Newtonian hydrodynamics. We found that the Poisson equation takes on a particular simple form, if the matter density fluctuation is expressed in the total matter gauge, and not the comoving orthogonal gauge which is used at first order. The difference of the two gauges only becomes apparent at second order in perturbation theory.

As an example, we calculate the second order Poisson equation in the case of an Einstein-de Sitter universe, and present the result in Eq. (4.4) in Fourier space. We show how to incorporate primordial non-Gaussianity into the matter perturbation at second order in an equation consistent with GR. In this way, we can also quantify the non-Gaussianity intrinsic to GR contributions. Our results generalise the non-Gaussian kernels presented in terms of Newtonian physics in Ref. [17] to include relativistic terms. We show that the non-linearity of GR induces a non-Gaussian signature on top of the primordial value. In particular we find, in the local configuration, a value  $f_{\text{NL}}^{loc(GR)} = -1$ . This is close to that obtained in Ref. [28], with the difference likely due to different gauges being used.

The general result, the Poisson equation at second order, and the example presented in this paper provide fairly simple equations that can be directly incorporated into generators of initial conditions for numerical simulations. The initial conditions generated in this way account for general relativistic effects in N-body codes and other numerical simulations of structure formation.



## Acknowledgements

JCH is grateful to Marc Manera for useful discussions. The authors are grateful for the support of the DGAPA-UNAM through the grant PAPIIT IN116210-3. AJC acknowledges support from the European Commission's Framework Programme 7, through the Marie Curie International Research Staff Exchange Scheme LACEGAL (PIRES-GA-2010-269264) and is grateful to the IA-UNAM, ICN-UNAM, and QMUL for hospitality. JCH is funded by CONACYT (CVU No. 46280), AJC by the Sir Norman Lockyer Fellowship of the Royal Astronomical Society, and KAM is supported, in part, by STFC grant ST/J001546/1.

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